Miniapplications: Vehicles for Co-design

SOS 15, Engelberg, Switzerland

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A Listing of Application Proxies

- Skeleton App:
  - Communication accurate, computation fake.
- Compact App:
  - A small version of a real app.
  - Attempting some tie to physics.
- Scalable Synthetic Compact Applications (SSCA):
  - DARPA HPCS.
  - Formal specification.
  - Code and detailed spec to allow re-write.

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App Proxies (cont).

- HPC Challenge Benchmarks.
- NAS Parallel Benchmarks.
- SPEC.
- HPL: Really?
  - Yes: In the ’80s
  - Approximated:
    - Frontal solver, NASTRAN, ANSYS, more.
    - Multifrontal/Supernodal solver: First Gordon Bell.
  - Question: Why are DCA++, LSMS fastest apps?
  - Answer (?): HPL was first co-design vehicle…
    that never died!

… And There are More: A crowded space

- UHPC Challenge Problems:
  - Formal specification.
  - Math, kernel extraction.
  - Intended to be open source?
- Motifs, aka dwarves.
  - Really are patterns, not actionable.

  "Even as cartoon characters they are sketchy."

  (John Lewis)

Question: Is there room for another approach?

Miniapps: Specs

- Size: O(1K) lines.
- Focus: Proxy for key app performance issue.
- Availability: Open Source.
- Scope of allowed change: Any and all.
- Intent: Co-design: From HW registers to app itself.
- Developer & owner: *Application team*.
- Lifespan: *Until it's no longer useful.*

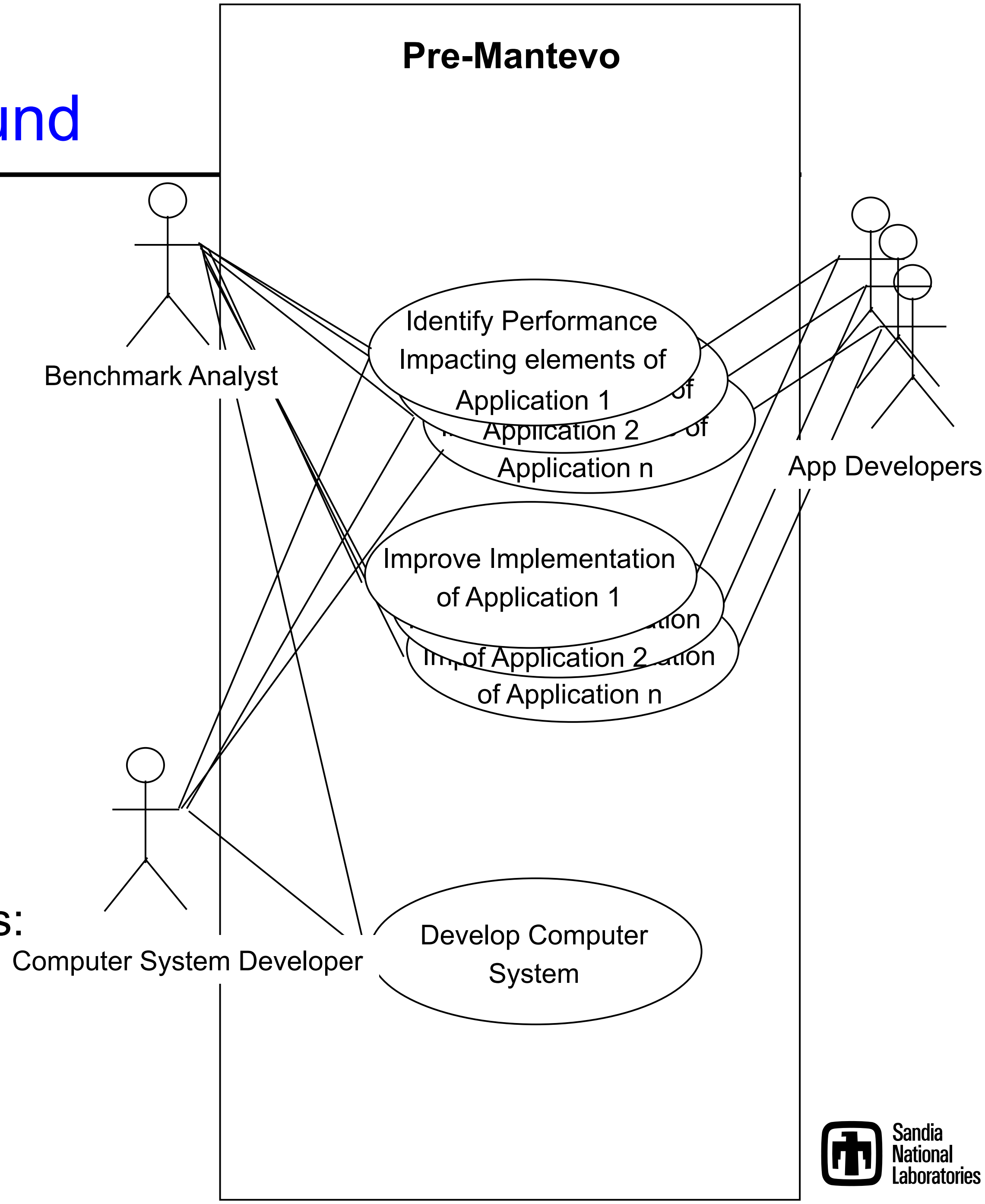
Mantevo* Project

* Greek: augur, guess, predict, presage

- Multi-faceted application performance project.
- Started 4 years ago.
- Two types of packages:
  - Miniapps: Small, self-contained programs.
    - MiniFE/HPCCG: unstructured implicit FEM/FVM.
    - phdMesh: explicit FEM, contact detection.
    - MiniMD: MD Force computations.
    - MiniXyce: Circuit RC ladder.
    - CTH-Comm: Data exchange pattern of CTH.
  - Minidrivers: Wrappers around Trilinos packages.
    - Beam: Intrepid+FEI+Trilinos solvers.
    - Epetra Benchmark Tests: Core Epetra kernels.
    - Dana Knoll working on new one.
- Open Source (LGPL)
- Staffing: Application & Library developers.

Background

- Goal: Develop scalable computing capabilities via:
  - Application analysis.
  - Application improvement.
  - Computer system design.
- Fixed timeline.
- Countless design decisions.
- Collaborative effort.
- Pre-Mantevo:
  - Work with each, large application.
  - Application developers have conflicting demands:
    - Features,
    - performance.
  - Application performance profiles have similarities.

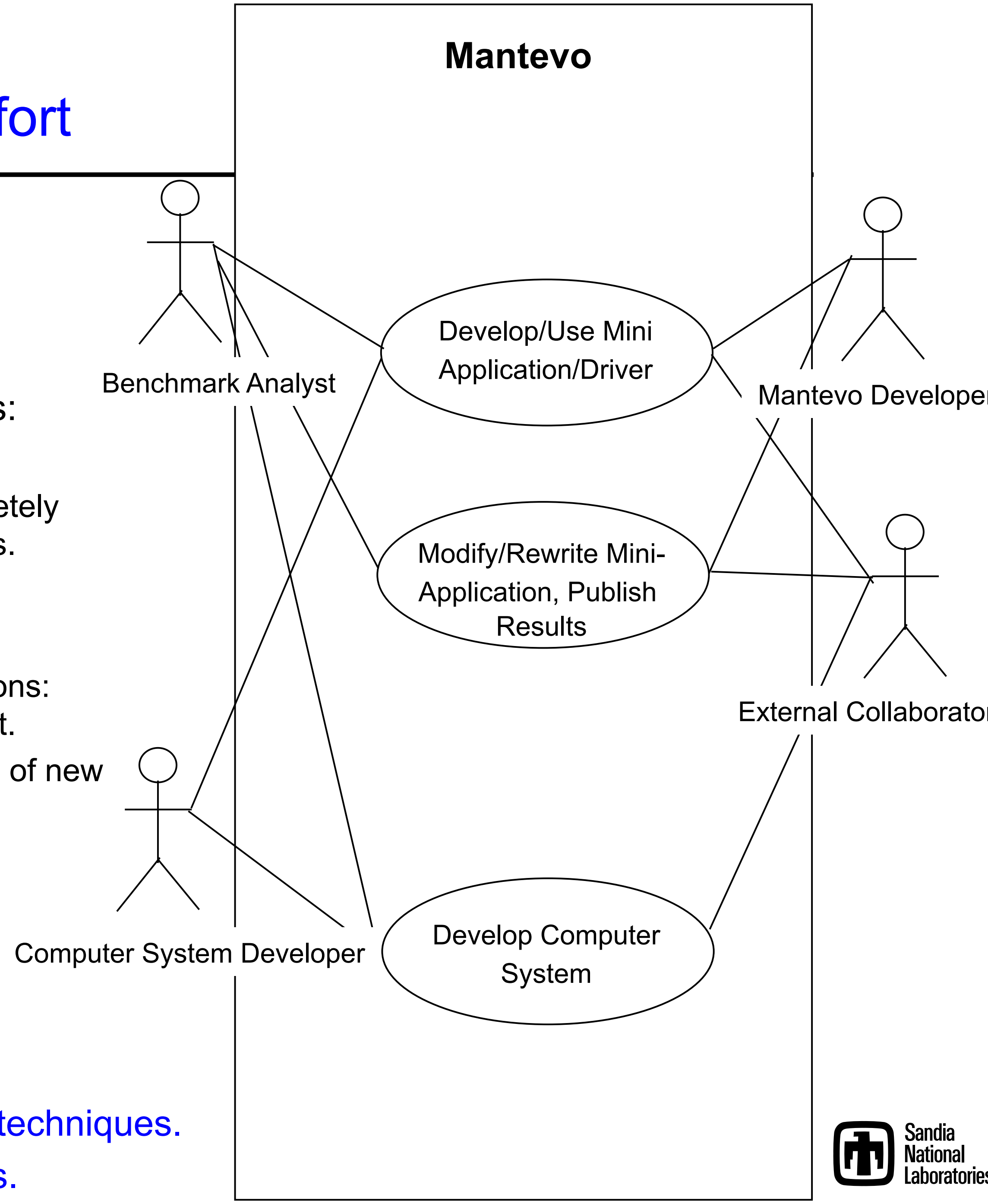


Mantevo Effort

- Develop:
  - Mini apps, mini drivers.
- Goals:
  - Aid in system design decisions:
    - Proxies for real apps.
    - Easy to use, modify or completely rewrite, e.g., multicore studies.
  - Guide application and library developers:
    - Get first results in new situations: apps/libs know what to expect.
    - Better algorithms: Exploration of new approaches.
  - Predict performance of real applications in new situations.
  - New collaborations.

Results:

- Better-informed design decision.
- Broad dissemination of optimization techniques.
- Incorporation of external R&D results.



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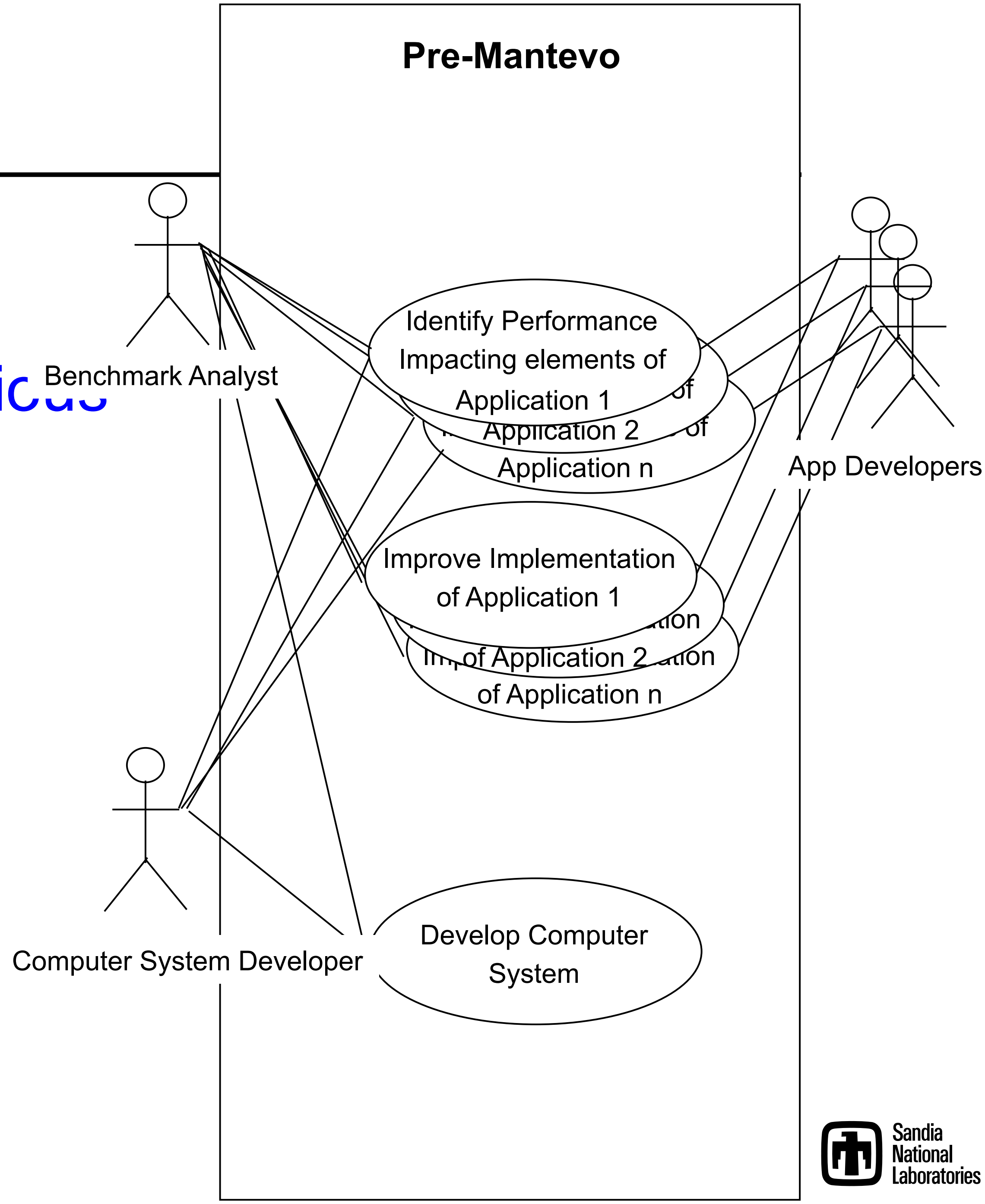
Didn’t give up on previous approach

Just added tools upstream



Examples

First Mantevo miniapp: HPCCG

- Glorified unstructured, distributed CG solve.
- SLOCCOUNT: 4091 SLOC (C++).
- Scalable (in z-dimension) to any processor count.
- Many targets:
  - Internode: MPI or not.
  - Intranode: Serial, OpenMP,
  - Scalar: float, double, complex
  - Int: 8, 16, 32, 64.
- Studied in numerous settings.

How could HPCCG really be a proxy?

- Simple logic experiment:
  - Many implicit apps spend 90+% of time in solver.
  - Solver is multi-level preconditioned Krylov method.
    - CG is (simple) Krylov method.
    - Preconditioner time dominated by smoother (GS, ILU)
    - GS, ILU similar to SpMV (except on multicore).
  - HPCCG is SpMV+CG.
- Can’t be accept results blindly.
  - App ownership of miniapp important here.

Data Placement on NUMA

- Memory Intensive computations: Page placement has huge impact.
- Most systems: First touch.
- Application data objects:
  - Phase 1: Construction phase, e.g., finite element assembly.
  - Phase 2: Use phase, e.g., linear solve.
- Problem: First touch difficult to control in phase 1.
- Idea: Page migration.
  - Not new: SGI Origin. Many old papers on topic.

Data placement experiments

- MiniApp: HPCCG
- Construct sparse linear system, solve with CG.
- Two modes:
  - Data placed by assembly, not migrated for NUMA
  - Data migrated using parallel access pattern of CG.
- 1 hour of effort to modify code.
- Results on dual socket quad-core Nehalem system.
- Migrate-on-next-touch:
  - RT/OS feature.
  - Study: Pedretti, Merritt, *Managing Shared Memory Data Distribution in Hybrid HPC Applications,* SAND2010-6262, Sep 2010.

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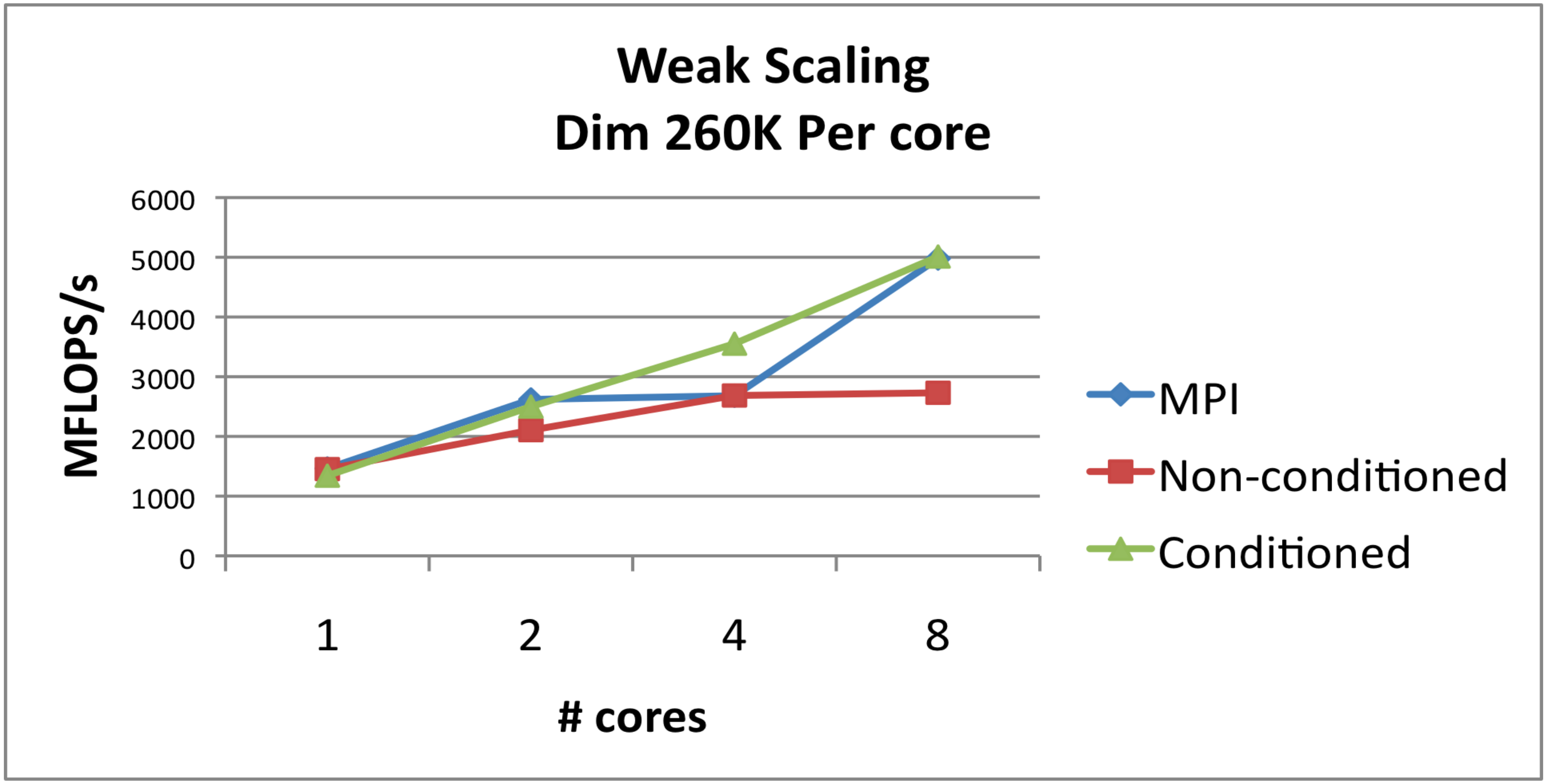
Weak Scaling Problem



- MPI and conditioned data approach comparable.
- Non-conditioned very poor scaling.

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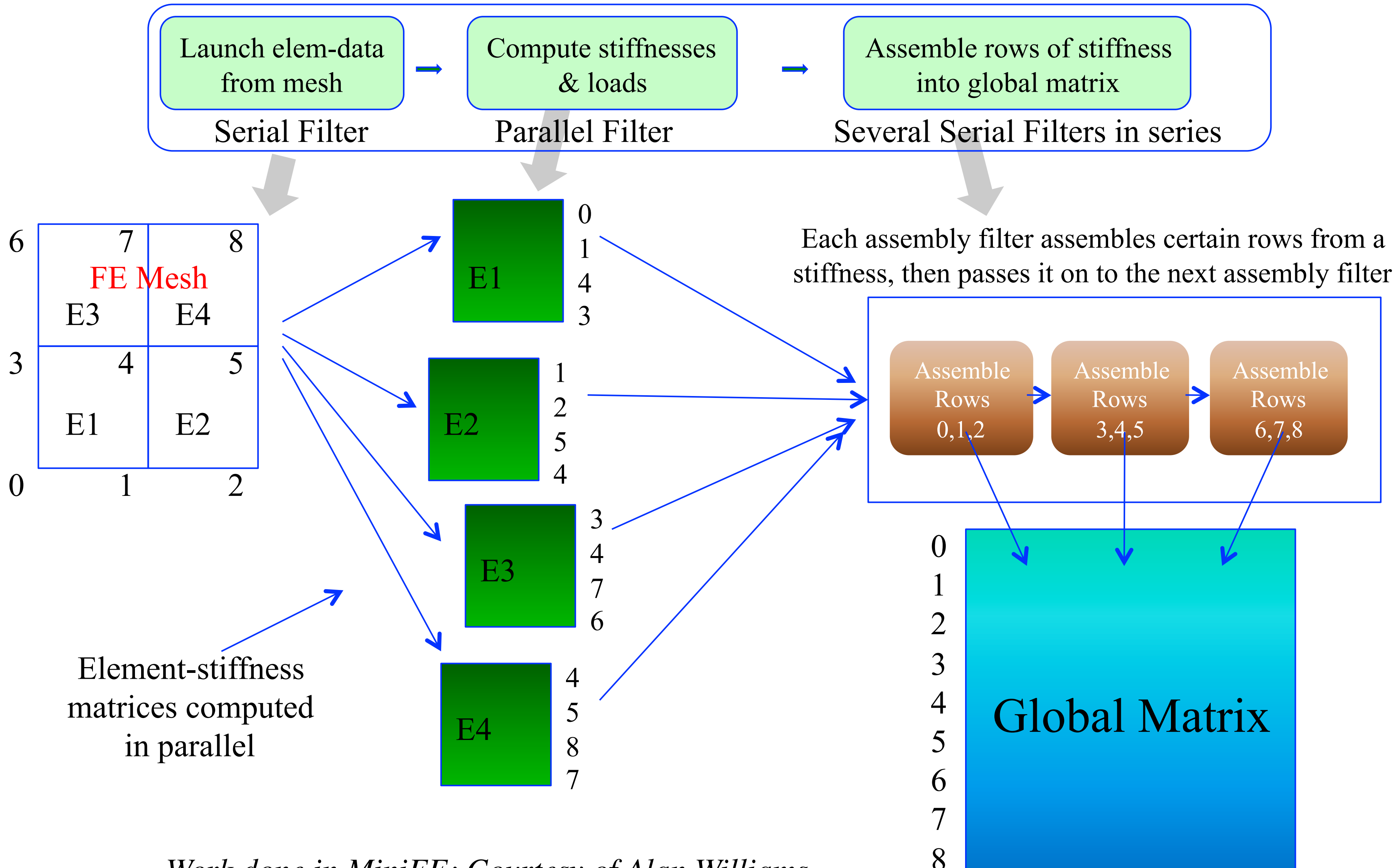
Much more…

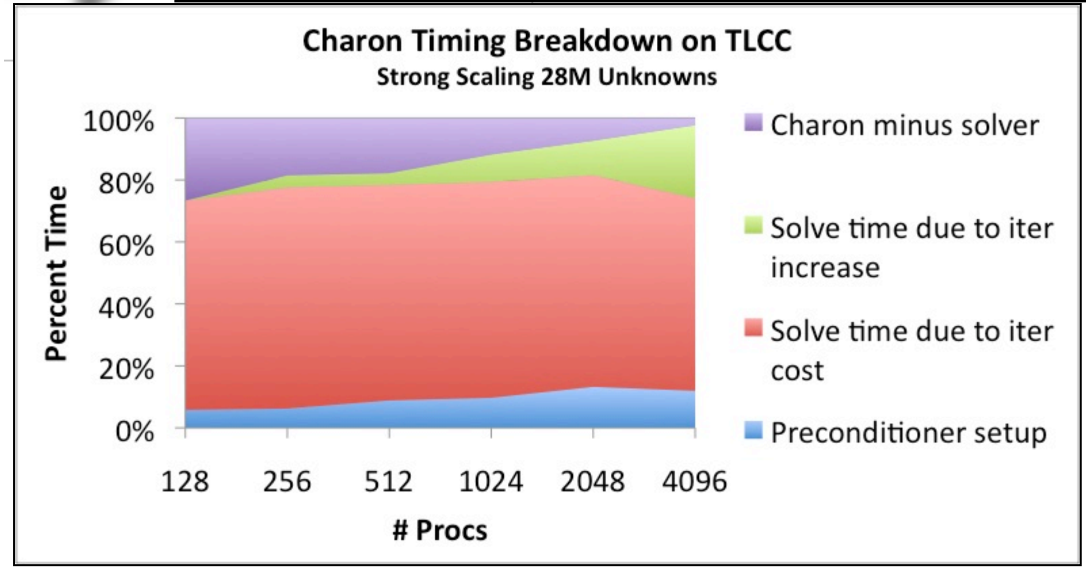
- Rewrites of HPCCG:
  - Pthreads, OpenMP, Chapel, qthreads…
- MiniFE:
  - Prototype of Kokkos Node API.
  - Prototype of pipeline and task graph node parallelism.
- Skeleton app of miniapp!
- Performance comparisons of different platforms:
  - All.

TBB Pipeline for FE assembly

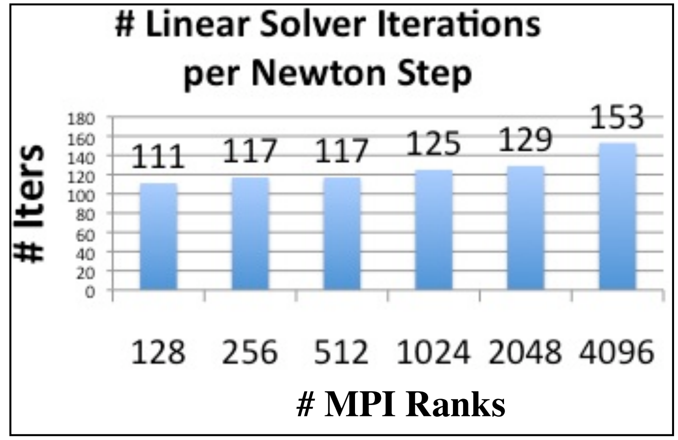


Work done in MiniFE: Courtesy of Alan Williams

Preconditioners for Scalable Multicore Systems



Strong scaling of Charon on TLCC (P. Lin, J. Shadid 2009)



- Observe: Iteration count increases with number of subdomains.
- With scalable threaded smoothers (LU, ILU, Gauss-Seidel):
  – Solve with fewer, larger subdomains.
  – Better kernel scaling (threads vs. MPI processes).
  – Better convergence, More robust.
- Exascale Potential: Tiled, pipelined implementation.
- Three efforts:
  – Level-scheduled triangular sweeps (ILU solve, Gauss-Seidel).
  – Decomposition by partitioning
  – Multithreaded direct factorization

MPI Tasks	Threads	Iterations
4096	1	153
2048	2	129
1024	4	125
512	8	117
256	16	117
128	32	111

Factors Impacting Performance of Multithreaded Sparse Triangular Solve, **Michael M. Wolf and Michael A. Heroux and Erik G. Boman, VECPAR 2010.**

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Emerging Abstract Machine Model: Thread team

- Multiple threads.
- Fast barrier.
- Shared, fast access memory pool.
- Required to address the constraints of global SIMT.
- Example: Nvidia SM
- X86 more vague, emerging more clearly in future.
- Prototyped in variant of HPCCG.

Managing Miniapp Data

Data Management
Common Look-and-Feel: YAML

- Input parameters:
  - Command line.
  - YAML file.
- Output:
  - YAML.
  - Embeds input parameters.
  - Output file can be input.
- Data parsing and collection:
  - Email list submission of YAML file.
  - CoPylot: Digests email, populates database.
- Common YAML data functions across all miniapps.

YAML ain't a Markup Language

- *de facto* standard format
- Human readable
- Convertible to/from XML, others

```
currentElement->get("performance_summary")->add("total","");
currentElement->get("performance_summary")->get("total")->add("time",times[0]);
currentElement->get("performance_summary")->get("total")->add("flops",3.0*fnops);
currentElement->get("performance_summary")->get("total")->add("mflops",3.0*fnops/times[0]/1.0E6);
```

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YAML Output File Excerpts

```
beefy.109% ./miniFE.x nx=30 ny=30 nz=30
 creating/filling mesh...0.00031209s, total time: 0.00031209
generating matrix structure...0.0196991s, total time: 0.0200112
        assembling FE data...
get-nodes: 0.0035727
compute-elems: 0.090822
sum-in: 0.0277233
0.125864s, total time: 0.145875
      imposing Dirichlet BC...0.0176551s, total time: 0.16353
making matrix indices local...8.10623e-06s, total time: 0.163538
Starting CG solver ...
Initial Residual = 182.699
Iteration = 5   Residual = 43.6016
Iteration = 10   Residual = 6.13924
Iteration = 15   Residual = 0.949901
Iteration = 20   Residual = 0.131992
Iteration = 25   Residual = 0.0196088

…
```


```
Platform:
  hostname: beefy.cs.csbsju.edu
  kernel name: 'Linux'
  kernel release: '2.6.34.7-66.fc13.x86_64'
  processor: 'x86_64'
Build:
  CXX: '/usr/lib64/openmpi/bin/mpicxx'
  compiler version: 'g++ (GCC) 4.4.5 20101112 (Red Hat
    4.4.5-2)'
  CXXFLAGS: '-O3'
  using MPI: yes
  Threading: none
Run Date/Time: 2011-03-14, 22-30-26
Rows-per-proc Load Imbalance:
  Largest (from avg, %): 0
  Std Dev (%): 0
…

Total:
    Total CG Time: 0.065695
    Total CG Flops: 9.45762e+07
    Total CG Mflops: 1439.63
  Time per iteration: 0.0013139
Total Program Time: 0.237604
```


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Emerging value: Broad Distribution
The Sentinel Dynamic

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Validation

Are Miniapps Predictive?

Does MiniFE Predict Charon Behavior? Processor Ranking: 8 MPI tasks; 31k DOF/core

- Charon steady-state drift-diffusion BJT
- Nehalem (Intel 11.0.081 –O2 –xsse4.2; all cores of dual-socket quadcore)
- 12-core Magny-Cours (Intel 11.0.081 –O2; one socket, 4 MPI tasks/die)
- Barcelona (Intel 11.1.064 –O2; use two sockets out of the quad-socket)
- 2D Charon (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ in matrix row
- Charon LS w/o or w/ ps: GMRES linear solve without/with ML precond setup time
- Try to compare MiniFE "assembling FE"+"imposing BC" time with Charon equivalent

MiniFE

	CG	FE assem+BC
1	Nehalem	Nehalem
2	MC(1.7)	MC(1.7)
3	Barc(2.7)	Barc(1.8)

Charon

	LS w/o ps	LS w/ ps	Mat+RHS
1	Nehalem	Nehalem	Nehalem
2	MC(1.7)	MC(1.8)	MC(1.46)
3	Barc(2.8)	Barc(2.5)	Barc(1.52)

Number in parenthesis is factor greater than #1 time

MiniFE Predict Charon? Multicore Efficiency Dual-Socket 12-core Magny-Cours : 124k DOF/core

- Charon steady-state drift-diffusion BJT; Intel 11.0.081 –O2
- Weak scaling study with 124k DOF/core
- 2D Charon (3 DOF/node) vs. 3D MiniFE; match DOF/core and NNZ in matrix row
- Efficiency: ratio of 4-core time to n-core time (expressed as percentage)
- Charon LS w/o or w/ ps: GMRES linear solve without/with ML precond setup time
- 100 Krylov iterations for both MiniFE and Charon (100 per Newton step)

MiniFE

cores	CG eff
4	Ref
8	89
12	73
16	61
20	54
24	45

Charon

cores	LS w/o ps eff	LS w/ ps eff
4	Ref	Ref
8	87	89
12	74	78
16	61	66
20	49	54
24	40	45

Miniapps Predictive?

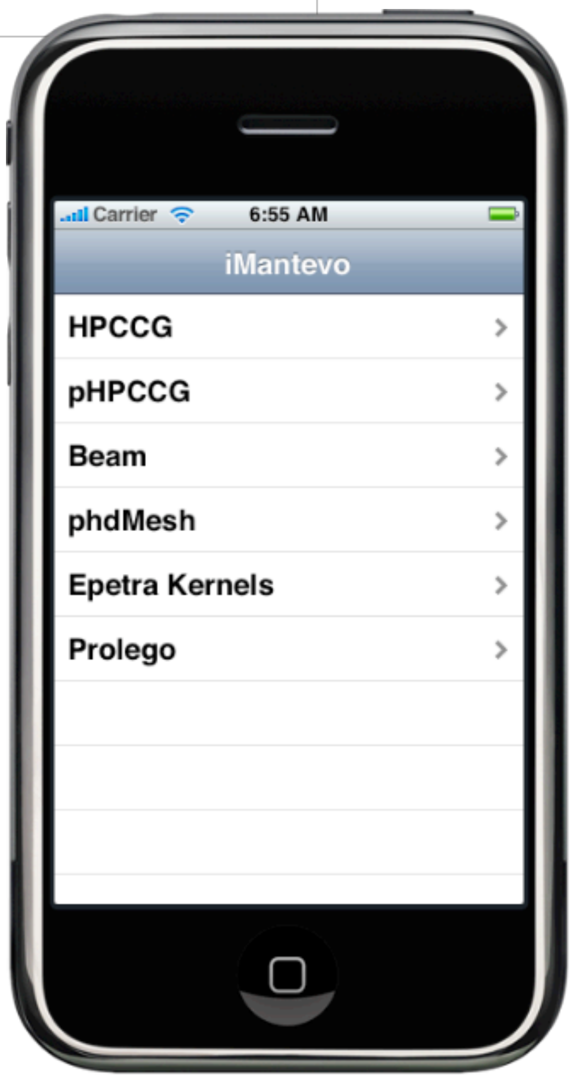
- First results are good:
  - No misleading trends.
- Careful calibration required: Apples to apples.
- Big plus: Ease of porting.

Charon Complexity

- SLOCCOUNT (tool from David A. Wheeler).
  - Charon physics: 191,877 SLOC.
  - Charon + nevada framework 414,885 SLOC
  - Charon_TPL 4,022,296 SLOC
- Library dependencies:
  - 25 Trilinos package.
  - 15 other TPLs.
- Requires “heroic effort” to build.
- MPI-only, no intranode parallelism.
- Export controlled.
- Stats courtesy of Roger Pawlowski.

MiniFE Complexity

- SLOCCOUNT:
  - Main code: 6,469 SLOC
  - Optional libraries (from Trilinos): 37,040 SLOC
- Easy to build:
  - Multiple targets:
    - Internode: MPI or not.
    - Intranode: Serial, Pthreads, OpenMP, TBB, CUDA.
  - Dialable properties:
    - Compute load imbalance.
    - Communication imbalance.
    - Data types: float, double, mixed.
- Open source.
- Stats: Courtesy of me.


Carrier
6:55 AM
iMantevo
HPCCG
pHPCCG
Beam
phdMesh
Epetra Kernels
Prolego


Carrier
6:56 AM
iMantevo
HPCCG
Nx = 75
Ny = 50
Nz = 50
Start
HPCCG Results:
(nx=75,ny=50,nz=50)
Total MFLOPS = 348.46
Press Start to run again.

Next Target App: CTH

- CTH:
  - Multi-material, large deformation, shock physics.
  - Used through DOE complex, heavily used by DOD.
- Each time step:
  - 2D face exchanges (19 times in each of 3 dims).
  - 1 face exchange: 40 arrays.
  - 100x100x100 local problem: 3.2 MB per face.
- Future systems (e.g. Cray Cielo):
  - Higher network injection rates.
- Goal: Study different comm algorithms to exploit rates.

Latest Miniapp: CTH Comm Proxy

- Miniapp: 2D face exchange with simple 27-pt computation.
- Explore spectrum of comm algorithms:
  - Standard approach as baseline.
  - Transmit each variable as soon as available.
  - Transmit as soon as any 2D slide is availabe.
- Introduce dialable load imbalance.
- Results?
  - See Richard Barrett's paper, submission to SC'11.

Summary

- Miniapps:
  - In many ways similar to other efforts.
  - Two important distinctions:
    - App team develops and owns.
    - Miniapp retired when no longer useful.
  - Some strengths:
    - Completely open process: LGPL, validation.
    - Highly collaborative.
- Challenges:
  - Engaging already-busy apps developers.
  - Keeping miniapps relevant over time (to avoid premature retirement).
- Mantevo site: http://software.sandia.gov/mantevo
- Soon: mantevo.org (website up, not populated)